Mathematics Methods and Thermodynamics

Kinetics III - Special Ordinary Differential Equations

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September 8, 2017

Class Overview

- Solving ODEs
- Special ODE functions
- Fourier Series

Review

- Ordinary Differential Equations (ODEs) are used in kinetics to solve the rates of complex reactions
- What are ODEs?
  - ODEs are equations with differentials and only one independent variable
- ODEs are classified as:
  - Linear: Where there are no powers of the function greater than one
  - Homogenous: Where the expression equates to zero
  - Order: This is the order of the highest order differential

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Solving ODEs

- Solving an ODE involves finding a function that satisfies the ODE
- For example the ODE

$$y' - 3y = 0$$

Is solved by the function

$$y = Ce^{3x}$$

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Solving ODEs

- We can test this by substituting back into the ODE

$$y = Ce^{3x}$$
$$y' = 3Ce^{3x}$$
$$3Ce^{3x} - 3Ce^{3x} = 0$$

Solving ODEs

- There are various techniques to solve ODEs depending on the nature of the ODE

Separation of Variables
: This technique is useful for simple functions were x and y can be separated

Integration
: Even if you cannot separate your function it is sometimes possible to integrate to achieve solution if it is of a satisfiable form

Integrating Factor
: Inexact derivatives need to be first converted to exact derivatives with an integrating factor. In addition some linear ODEs can be solved with an integrating factor.

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Solving ODEs: Separation of Variables

- Separation of variables is done when you have a function that can be represented as:

$$\frac{dy}{dx} = F(y)$$

In this case it is solved by

$$\int \frac{1}{F(y)}\, dy = \int 1\, dx$$

Solving ODEs: Separation of Variables

- If your function can be separated into x and y as in the following
$$F(y)\frac{dy}{dx} + G(x) = 0$$
Then you can directly integrate
$$\int F(y)\,dy + \int F(x)\,dx = C$$

Solving ODEs: Direct Integration

- In some cases you can directly integrate to solve an ODE
- If it is first order and of the form

$$F(x,y)\frac{dy}{dx} + G(x,y) = 0$$

as long as $\frac{dF}{dy} = \frac{dG}{dx}$ then it can be integrated as:

$$\int F(x,y)\,dy + \int G(x,y)\,dx + Y(y) + X(x) = C$$

where $Y(y)$, $X(x)$ and C are set to satisfy the initial conditions.

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Solving ODEs: Integrating Factor

- Previously we learned that inexact differentials have no anti-derivative
- This means we cannot solve the ODE which depends upon integration
- However for any inexact differential of two variable there exists an integrating factor that converts it to an exact differential

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Inexact Differential

- What is an inexact differential?
- It is a differential where the path taken changes the result
- In practice this means that making a small change in y then making a small change in x will give a different result that the reverse

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Solving ODEs: Integrating Factor

- After rearranging your expression to something of the form

$$F(x,y)\,dx + G(x,y)\,dy = 0$$

- If you find that $\frac{dF}{dy} \neq \frac{dG}{dx}]$ then it is an inexact differential
- To integrate the expression we must find an integrating factor μ such that

$$\frac{dF}{dy}\mu + \frac{d\mu}{dy} = \frac{dG}{dx}\mu + \frac{d\mu}{dx}$$

  Although this looks like another differential equation it is not. Because it has two independent variables it is instead a partial differential equation
- These are notoriously difficult to solve and so it is hard to identify the integrating factor except in two cases

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Solving ODEs: Integrating Factor

- Integrating factors are easier to find in these two cases

Case 1 If the following expression is only a function of x (all the y's cancel):

$$\frac{\frac{dF}{dy} - \frac{dG}{dx}}{G}$$

Then the integrating factor is:

$$\mu = e^{\int \frac{\frac{dF}{dy} - \frac{dG}{dx}}{G} \, dx}$$

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Case 2 If the following expression is only a function of y (all the x's cancel):

$$\frac{-\frac{dF}{dy} + \frac{dG}{dx}}{F}$$

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Solving ODEs: Integrating Factor

- If you have a linear ODE of the form

$$\frac{dy}{dx} + F(x)y = Q(x)$$

- Then the integrating factor is

$$\mu = e^{\int F(x)\, dx}$$

- In this case we can write the general form of the answer as

$$y = \frac{1}{\mu}\left(\int \mu Q(x)\, dx + C\right)$$

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Special ODEs

- ODEs can be particularly difficult to solve especially in general form
- When an ODE is solved exactly in a general form it can be useful and is typically named after the discoverer
- For example we have solutions to ODEs discovered by
  - Laguerre
  - Lengendre
  - Hermite
  - Eckart
  - Euler
  - Jacobi
- Each of which have their own polynomials which are solutions to particular ODEs

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Special ODEs

- These polynomial are special functions that solve the ODE in a general way where some part is left variable
- For example associated Laguerre polynomials solve Laguerre differential equation

$$xy'' + (\nu + 1 - x)y' + \lambda y = 0$$

  Where λ and ν are real numbers that can be changed
- Sometimes there is more than one possible solution. There are for example infinite solutions for the Laguerre differential equation and consequently infinite Laguerre polynomials ($L_n^\nu(x)$)

$$L_n^\nu(x) = \frac{1}{n!}\sum_{i=0}^{n}\frac{n!}{i!}\binom{\nu+n}{n-i}(-x)^i$$

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Special ODEs: Laguerre

- The Laguerre ODE is

$$xy'' + (1 - x) + ny$$

- In its more general form it is the associated Laguerre polynomial

$$xy'' + (\nu + 1 - x) + ny$$

- To solve this expression we must use the integrating factor

$$\mu = \mathrm{e}^{\int \frac{\nu+1-x}{x}} = \mathrm{e}^{(\nu+1)\ln(x)-x} = x^{\nu+1}\mathrm{e}^{-x}$$

- After multiply the differential equation though by the integrating factor the expression become solvable and yields the Laguerre polynomial

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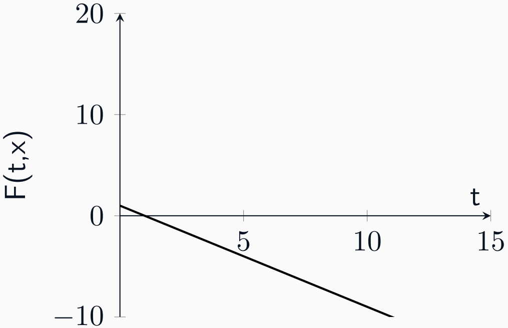
Special ODEs: Laguerre

- The first few Laguerre polynomials have the following form



$$n = 1 \qquad L_1^0(x) = -x + 1$$

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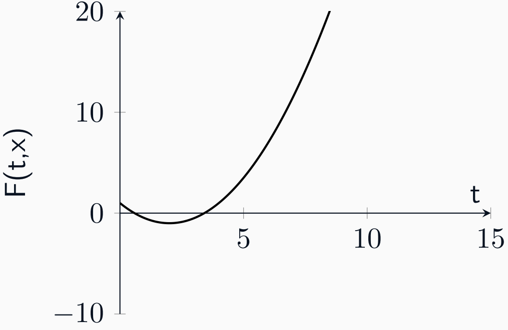

$$n = 2 \qquad L_2^0(x) = \frac{1}{2}\left(x^2 - 4x + 2\right)$$

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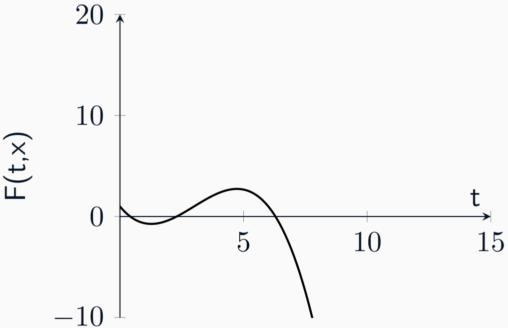

$$n = 3 \qquad L_3^0(x) = \frac{1}{6}\left(-x^3 + 9x^2 - 18x + 6\right)$$

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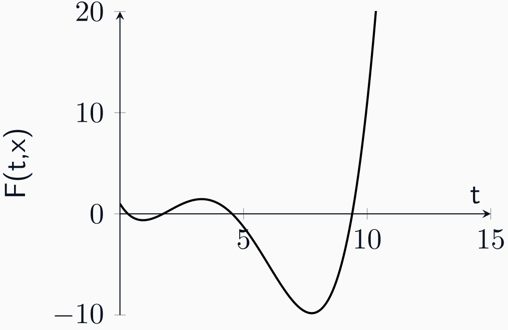

$$n = 4 \qquad L_4^0(x) = \frac{1}{24}\left(x^4 - 16x^3 + 72x^2 - 96x + 24\right)$$

Special ODEs: Laguerre

- The Laguerre polynomials are useful particularly in quantum mechanics as
  - They are an exact solution to the radial wavefunction of hydrogen
  - They have a set of recursion relations that when combined with its orthogonality condition make the integrals very easy to solve

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Special ODEs: Legendre

- Legendres differential equation is

$$\left(1-x^2\right)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+n\left(n+1\right)y=0$$

- It can also be written as

$$\frac{d}{dx}\left(\left(1-x^2\right)\frac{dy}{dx}\right)+n\left(n+1\right)y=0$$

- The more general form is the associate Legendre differential equation

$$\frac{d}{dx}\left(\left(1-x^2\right)\frac{dy}{dx}\right)+n\left(\left(n+1\right)-\frac{m^2}{1-x^2}\right)y=0$$

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Special ODEs: Legendre

- The solution is found by series expansion to be

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left(\left(x^2 - 1 \right)^n \right)$$

- With the associated solution being defined using the unassociated

$$P_n^m(x) = (-1)^2 \left(1 - x^2\right)^{m/2} \frac{d^m}{dx^m} \left(P_n(x)\right)$$

- They are valid in the range of -1 to 1

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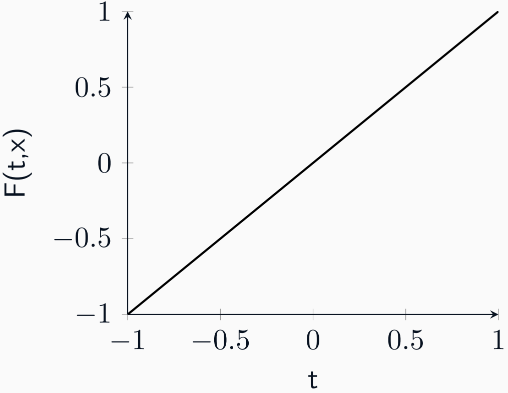

$$n = 1 \qquad P_1^0(x) = x$$

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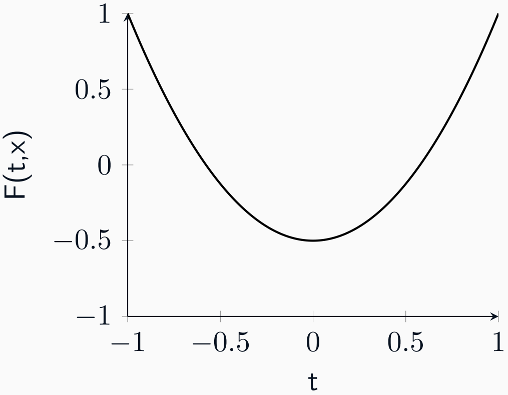

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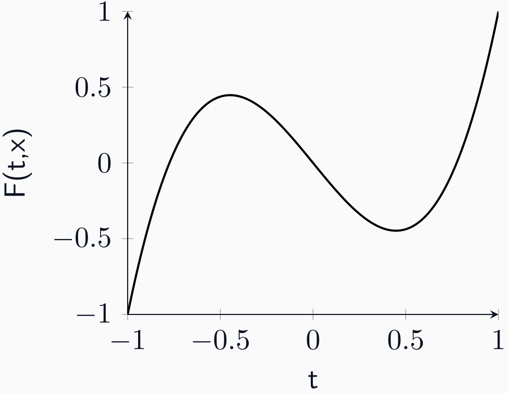

$$n = 3 \qquad P_3^0(x) = \frac{1}{2}\left(5x^3 - 3x\right)$$

Special ODEs: Legendre

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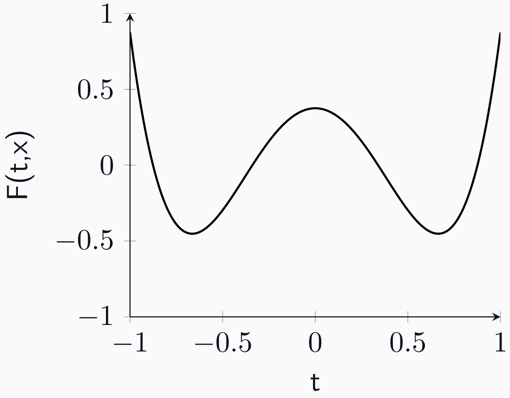

$$n = 4 \qquad P_4^0(x) = \frac{1}{8}\left(35x^4 - 30x + 3\right)$$

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  - In solving the Newtonian potential
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- The solution for the Hermite differential equation is

$$H_n(x) = n! \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(-1)^m}{m!\,(n-2m)!}\,(2x)^{n-2m}$$

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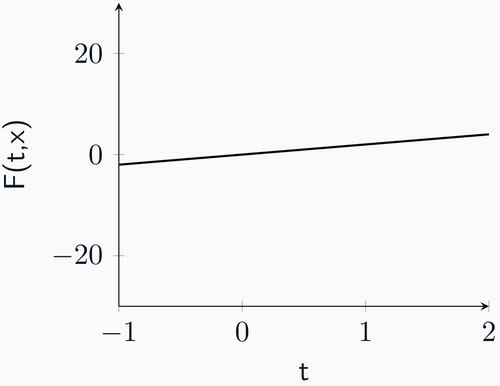

$$n = 1 \qquad H_1^0(x) = 2x$$

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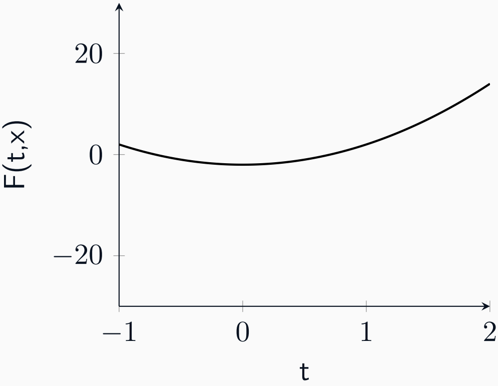

$$n = 2 \qquad H_2^0(x) = 4x^2 - 2$$

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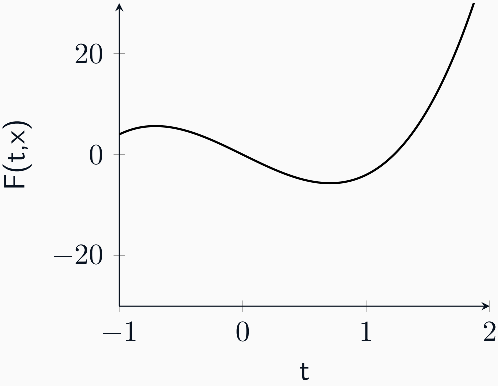

$$n = 3 \qquad H_3^0(x) = 8x^3 - 12x$$

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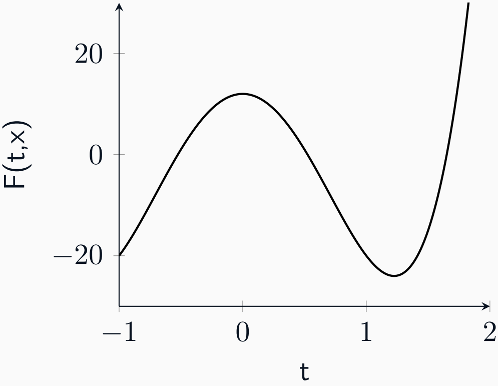

$$n = 4 \qquad H_4^0(x) = 16x^4 - 48x^2 + 12$$

Special ODEs: Hermite

- Hermite polynomials although look particularly complex are useful in that they satisfy the equation

$$y'' + \left(2n + 1 - x^2\right) y = 0$$

  This is the Schrödinger equation for the harmonic oscillator. This is used in QM to calculate your frequencies and therefore to approximate your thermal, enthalpy and Gibbs energies
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Special ODEs: Summary

- Special ODEs are well known exact ODEs that are of particular importance due to their generality and uses
- There are many special ODEs but the most useful in Chemistry are perhaps:

  Laguerre The solutions of which give the radial hydrogenic wavefunction. They range from zero to infinity

  Legendre The solutions of which give the angular hydrogenic wavefunction, and Newtons potentials. They range from -1 to 1

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Fourier Series

- There are times when it is difficult to represent some function in a useful manner instead we want to approximate that function
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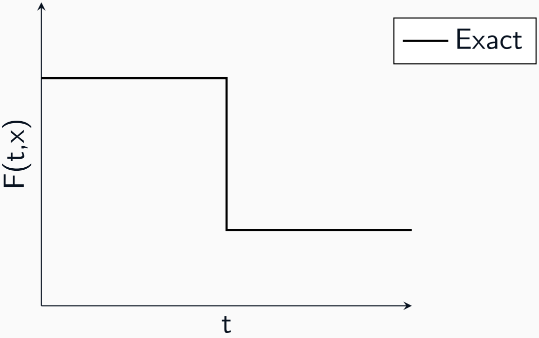

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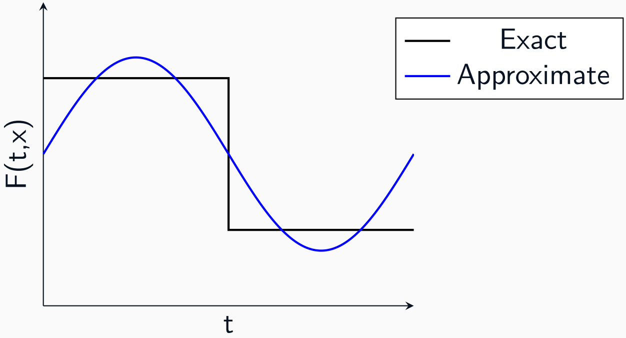

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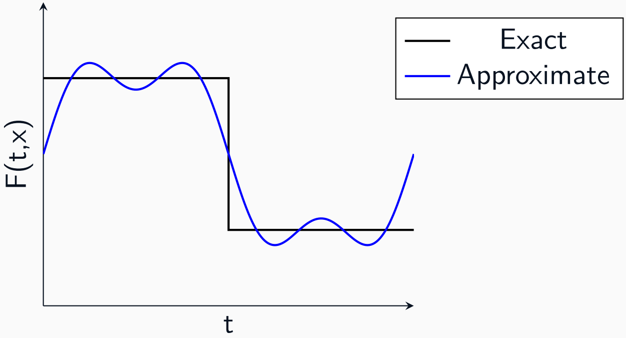
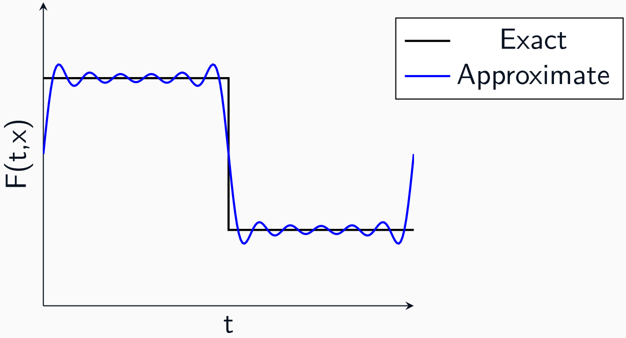
Fourier Series: Square Wave



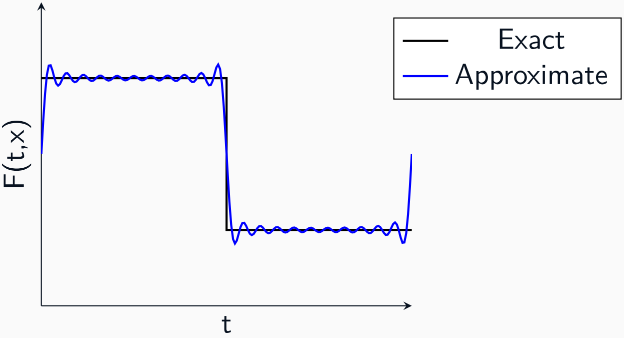
$n = 2$

Fourier Series: Square Wave



$n = 5$

Fourier Series: Square Wave



$n = 10$

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- While it converges to the midpoint between discontinuous points

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$$\int_{-\pi}^{\pi} \sin(mx)\sin(nx)\, dx = \pi\delta_{m,n} \qquad \text{For } m, n \neq 0$$

$$\int_{-\pi}^{\pi} \cos(mx)\cos(nx)\, dx = \pi\delta_{m,n} \qquad \text{For } m, n \neq 0$$

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- We then expand our arbitrary function into the Fourier series

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(nx) + \sum_{n=1}^{\infty} b_n \sin(nx)$$

After applying a coordinate transform such that the area of interest is between $-\pi$ and π

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- By using this we can compute all the coefficients in the expansion

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- We discussed methods for solving ODEs analytically including
  - Separation of Variables
  - Direct Integration
  - Integrating factor
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